

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:ssptayvv1621

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

***** Welcome to STN International *****

NEWS 1 Web Page for STN Seminar Schedule - N. America
NEWS 2 OCT 02 CA/CAPLUS enhanced with pre-1907 records from Chemisches
Zentralblatt
NEWS 3 OCT 19 BEILSTEIN updated with new compounds
NEWS 4 NOV 15 Derwent Indian patent publication number format enhanced
NEWS 5 NOV 19 WPIX enhanced with XML display format
NEWS 6 NOV 30 ICSD reloaded with enhancements
NEWS 7 DEC 04 LINPADOCDB now available on STN
NEWS 8 DEC 14 BEILSTEIN pricing structure to change
NEWS 9 DEC 17 USPATOLD added to additional database clusters
NEWS 10 DEC 17 IMSDRUGCONF removed from database clusters and STN
NEWS 11 DEC 17 DGENE now includes more than 10 million sequences
NEWS 12 DEC 17 TOXCENTER enhanced with 2008 MeSH vocabulary in
MEDLINE segment
NEWS 13 DEC 17 MEDLINE and LMEDELINE updated with 2008 MeSH vocabulary
NEWS 14 DEC 17 CA/CAPLUS enhanced with new custom IPC display formats
NEWS 15 DEC 17 STN Viewer enhanced with full-text patent content
from USPATOLD
NEWS 16 JAN 02 STN pricing information for 2008 now available
NEWS 17 JAN 16 CAS patent coverage enhanced to include exemplified
prophetic substances
NEWS 18 JAN 28 USPATFULL, USPAT2, and USPATOLD enhanced with new
custom IPC display formats
NEWS 19 JAN 28 MARPAT searching enhanced
NEWS 20 JAN 28 USGENE now provides USPTO sequence data within 3 days
of publication
NEWS 21 JAN 28 TOXCENTER enhanced with reloaded MEDLINE segment
NEWS 22 JAN 28 MEDLINE and LMEDELINE reloaded with enhancements
NEWS 23 FEB 08 STN Express, Version 8.3, now available
NEWS 24 FEB 20 PCI now available as a replacement to DPCI
NEWS 25 FEB 25 IFIREF reloaded with enhancements
NEWS 26 FEB 25 IMSPRODUCT reloaded with enhancements

NEWS EXPRESS FEBRUARY 08 CURRENT WINDOWS VERSION IS V8.3,
AND CURRENT DISCOVER FILE IS DATED 20 FEBRUARY 2008

NEWS HOURS STN Operating Hours Plus Help Desk Availability
NEWS LOGIN Welcome Banner and News Items
NEWS IPC8 For general information regarding STN implementation of IPC 8

Enter NEWS followed by the item number or name to see news on that
specific topic.

All use of STN is subject to the provisions of the STN Customer
agreement. Please note that this agreement limits use to scientific
research. Use for software development or design or implementation

of commercial gateways or other similar uses is prohibited and may result in loss of user privileges and other penalties.

* * * * * STN Columbus * * * * *

FILE 'HOME' ENTERED AT 15:25:20 ON 25 FEB 2008

=> file reg

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

0.21

0.21

FILE 'REGISTRY' ENTERED AT 15:25:35 ON 25 FEB 2008

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

COPYRIGHT (C) 2008 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 24 FEB 2008 HIGHEST RN 1005323-41-0

DICTIONARY FILE UPDATES: 24 FEB 2008 HIGHEST RN 1005323-41-0

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 9, 2008.

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stdoc/properties.html>

=>

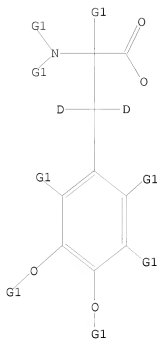
Uploading C:\Program Files\Stnexp\Queries\10539845-broad.str

L1 STRUCTURE UPLOADED

=> d l1

L1 HAS NO ANSWERS

L1 STR



G1 H,D

Structure attributes must be viewed using STN Express query preparation.

=> s l1

SAMPLE SEARCH INITIATED 15:25:57 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 848 TO ITERATE

100.0% PROCESSED 848 ITERATIONS

2 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 15213 TO 18707

PROJECTED ANSWERS: 2 TO 124

L2 2 SEA SSS SAM L1

=> s l1 full

FULL SEARCH INITIATED 15:26:02 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 16612 TO ITERATE

100.0% PROCESSED 16612 ITERATIONS

71 ANSWERS

SEARCH TIME: 00.00.01

L3 71 SEA SSS FUL L1

=> d l3 scan

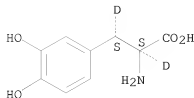
L3 71 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN

IN L-Tyrosine- α,β -d2, 3-hydroxy-, (BS)-

MF C9 H9 D2 N O4

CI COM

Absolute stereochemistry.



HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> file caplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

178.82

179.03

FILE 'CAPLUS' ENTERED AT 15:26:32 ON 25 FEB 2008

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

COPYRIGHT (C) 2008 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications. The CA Lexicon is the copyrighted intellectual property of the American Chemical Society and is provided to assist you in searching databases on STN. Any dissemination, distribution, copying, or storing of this information, without the prior written consent of CAS, is strictly prohibited.

FILE COVERS 1907 - 25 Feb 2008 VOL 148 ISS 9

FILE LAST UPDATED: 24 Feb 2008 (20080224/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

<http://www.cas.org/infopolicy.html>

=> s 13

L4 23 L3

=> s 14 not py > 2003

5375704 PY > 2003

L5 21 L4 NOT PY > 2003

=> d 15 ibib abs hitstr 1-

YOU HAVE REQUESTED DATA FROM 21 ANSWERS - CONTINUE? Y/(N):y

L5 ANSWER 1 OF 21 CAPLUS COPYRIGHT 2008 ACS ON STN

ACCESSION NUMBER: 2000:357850 CAPLUS

DOCUMENT NUMBER: 133:129208

TITLE: EPR Studies of Chromium(V) Intermediates Generated via Reduction of Chromium(VI) by DOPA and Related Catecholamines: Potential Role for Oxidized Amino Acids in Chromium-Induced Cancers

AUTHOR(S): Pattison, David I.; Lay, Peter A.; Davies, Michael J.
CORPORATE SOURCE: School of Chemistry, University of Sydney, Sydney, 2006, Australia

SOURCE: Inorganic Chemistry (2000), 39(13), 2729-2739
CODEN: INOCAJ; ISSN: 0020-1669

PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The redns. of K₂Cr₂O₇ by catecholamines, DOPA, DOPA- β , β -d₂, N-acetyl-DOPA, α -methyl-DOPA, dopamine, adrenaline, noradrenaline, catechol, 3,4-dihydroxybenzoic acid (DHBA), and 4-tert-butylcatechol (TBC), produce a number of Cr(V) EPR signals. These species are of interest in relation to the potential role of oxidized proteins and amino acids in Cr-induced cancers. With excess organic ligand, all of the substrates yield Cr species with signals at giso .apprx. 1.972 (Aiso(53Cr) > 23.9 + 10⁻⁴ cm⁻¹). These are similar to signals reported previously but were reassigned as octahedral Cr(V) species with mixed catechol-derived ligands, [CrV(semiquinone)2(catecholate)]⁺. Expts. with excess K₂Cr₂O₇ show complex behavior with the catecholamines and TBC. Several weak Cr(V) signals are detected after mixing, and the spectra evolve over time to yield relatively stable substrate-dependent signals at giso .apprx. 1.980. These signals were attributed to [Cr(O)L₂]- (L = diolato) species, in which the Cr is coordinated to two cyclized catecholamine ligands and an oxo ligand. Isotopic labeling studies with DOPA (ring or side chain deuteration or enrichment with ¹⁵N), and simulation of the signals, show that the superhyperfine couplings originate from the side chain protons, confirming that the catecholamine ligands are cyclized. At pH 3.5, a major short-lived EPR signal is observed for many of the substrates at giso .apprx. 1.969, but the species responsible for this signal was not identified. Several other minor Cr signals are detected, which are attributed (by comparison with isoelectronic V(IV) species) to Cr(V) complexes coordinated by a single catecholamine ligand (and auxiliary ligands e.g. H₂O), or to [Cr(O)L₂]- (L = diolato) species with a 6th ligand (e.g. H₂O). Addition of catalase or deoxygenation of the solns. did not affect the main EPR signals. When the substrates were in excess (pH > 4.5), primary and secondary (cyclized) semiquinones were also detected. Semiquinone stabilization by Zn(II) complexation yielded stronger EPR signals (giso .apprx. 2.004).

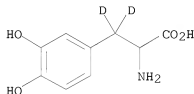
IT 27313-66-2D, chromium(V) complexes of derivs.

RL: FMU (Formation, unclassified); PRP (Properties); FORM (Formation, nonpreparative)

(ESR study of chromium(V) intermediates and potential role for oxidized amino acids in chromium-induced cancers)

RN 27313-66-2 CAPLUS

CN Tyrosine- β , β -d₂, 3-hydroxy- (9CI) (CA INDEX NAME)



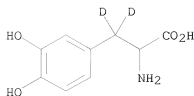
IT 27313-66-2

RL: RCT (Reactant); RACT (Reactant or reagent)

(reduction of chromium(VI) by DOPA and related catecholamines in ESR study of chromium(V) intermediates and potential role for oxidized amino acids in chromium-induced cancers)

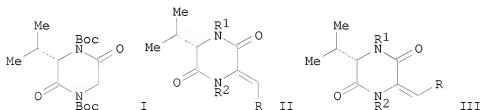
RN 27313-66-2 CAPLUS

CN Tyrosine- β , β -d₂, 3-hydroxy- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 77 THERE ARE 77 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

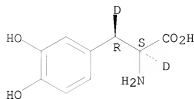
L5 ANSWER 2 OF 21 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1998:172416 CAPLUS
 DOCUMENT NUMBER: 128:283042
 TITLE: Stereo-divergent synthesis of L-threo- and L-erythro-[2,3-2H2]amino acids using optically active dioxopiperazine as a chiral template
 AUTHOR(S): Oba, Makoto; Terauchi, Tsutomu; Owari, Yuki; Imai, Yoko; Motoyama, Izumi; Nishiyama, Kozaburo
 CORPORATE SOURCE: Department of Material Science and Technology, Tokai University, Shizuoka, 410-03, Japan
 SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1998), (7), 1275-1282
 CODEN: JCPRB4; ISSN: 0300-922X
 PUBLISHER: Royal Society of Chemistry
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 128:283042
 GI



AB A stereodivergent synthesis of L-threo- and L-erythro-[2,3-2H2]amino acids from the same chiral auxiliary is described. Aldolization of protected dioxopiperazine I (Boc = CO₂Me₃), derived from L-valine, with various aldehydes RCHO [R1 = Ph, 4-MeOC₆H₄, 3,4-(MeO)₂C₆H₃, Me₂CD] followed by successive elaboration gives various 2,3-dehydroamino acid derivs II and III (R1 = R2 = H, Boc; R1 = Boc, R2 = H, Ac; R1 = Ac, R2 = Ac, Boc). Catalytic deuteration of II and III followed by acidic hydrolysis affords L-[2,3-2H2]amino acids in good yields with high optical purities. It becomes clear that diastereoselective deuteration for either the threo or the erythro isomer depends upon the protective groups on the nitrogen atoms in the dioxopiperazine ring. Thus, catalytic deuteration of II (R1 = R2 = Boc) gave 74% L-erythro-[2,3-2H2]phenylalanine with 98% e.e., while catalytic deuteration of II (R1 = R2 = H) gave 85% L-threo-[2,3-2H2]phenylalanine with 91% e.e.
 IT 205816-63-3P 205816-64-4P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (stereodivergent preparation of deuterated amino acids using chiral dioxopiperazine templates)
 RN 205816-63-3 CAPLUS

CN L-Tyrosine- α,β -d₂, 3-hydroxy-, (β R)- (CA INDEX NAME)

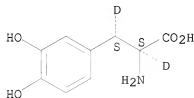
Absolute stereochemistry.



RN 205816-64-4 CAPLUS

CN L-Tyrosine- α,β -d₂, 3-hydroxy-, (β S)- (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 3 OF 21 CAPLUS COPYRIGHT 2008 ACS ON STN

ACCESSION NUMBER: 1994:260260 CAPLUS

DOCUMENT NUMBER: 120:260260

TITLE: Quantitative analysis of low molecular weight compounds of biological interest by matrix-assisted laser desorption ionization

AUTHOR(S): Duncan, Mark W.; Matanovic, Gabrijela; Cerpa-Poljak, Anne

CORPORATE SOURCE: Biomed. Mass Spectrometry Unit, Univ. New South Wales, Kensington, 2033, Australia

SOURCE: Rapid Communications in Mass Spectrometry (1993), 7(12), 1090-4

CODEN: RCMSEF; ISSN: 0951-4198

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Internal stds. were used to demonstrate that matrix-assisted laser desorption/ionization (MALDI) mass spectrometry can be applied to the quant. anal. of low mol. weight polar compds. Three examples were tested: a standard curve for 3,4-dihydroxyphenylalanine (DOPA) was prepared using a stable

isotope analog (i.e., [13C₆]DOPA) as an internal standard; [2H₁₆]-acetylcholine was employed as an internal standard for the quantification of acetylcholine; and in the final example, the peptide Ac-Ser-Ile-Arg-His-Tyr-NH₂ was used as an internal standard for the quantification of the peptide H-Ser-Ala-Leu-Arg-His-Tyr-NH₂. In each instance, straight line fits ($r^2 > 0.95$) demonstrate that MALDI is a viable approach for the quant. anal. of low mol. weight analytes.

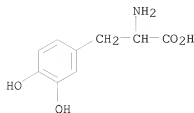
IT 154607-42-8

RL: ANST (Analytical study)

(as internal standard for determination of dihydroxyphenylalanine by matrix-assisted laser desorption ionization mass spectrometry)

RN 154607-42-8 CAPLUS

CN Tyrosine-13C₆, 3-hydroxy- (9CI) (CA INDEX NAME)



L5 ANSWER 4 OF 21 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1991:118039 CAPLUS

DOCUMENT NUMBER: 114:118039

TITLE: Fast enzymic preparation of L-DOPA from tyrosine and molecular oxygen: a potential method for preparing [oxygen-15]L-DOPA

AUTHOR(S): Maddaluno, Jacques F.; Faull, Kym F.

CORPORATE SOURCE: Sch. Med., Stanford Univ., Stanford, CA, 94305, USA

SOURCE: Applied Radiation and Isotopes (1990), 41(9), 873-8

CODEN: ARISEF; ISSN: 0883-2889

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A fast, simple, and inexpensive enzymic preparation of L-DOPA from mol. oxygen and tyrosine using mushroom tyrosinase is described. The theor. incubation time for production of [15O]L-DOPA with maximal specific activity from [15O]O2 can be calculated to be about 3 min. In practice, using a specially designed glass reaction chamber to facilitate the incorporation of gaseous mol. oxygen into L-DOPA with zero lag-time, a 3-min reaction with 1% oxygen in nitrogen results in the formation of approx. 3.9 μmol of L-DOPA, representing conversion of about 14% of the tyrosine substrate. Given access to a supply of [15O]O2, the method should be applicable to the preparation of [15O]L-DOPA for use as a PET tracer.

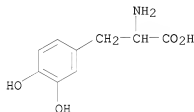
IT 132587-87-2P, preparation

RL: PREP (Preparation)

(preparation of, enzymic)

RN 132587-87-2 CAPLUS

CN L-Tyrosine, 3-hydroxy-, labeled with oxygen-15 (9CI) (CA INDEX NAME)



L5 ANSWER 5 OF 21 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1990:508668 CAPLUS

DOCUMENT NUMBER: 113:108668

TITLE: Comparative in vivo metabolism of 6-[18F]fluoro-L-DOPA and [3H]L-DOPA in rats

AUTHOR(S): Melega, William P.; Luxen, Andre; Perlmutter, Milton

M.; Nissenson, Charna H. K.; Phelps, Michael E.; Barrio, Jorge R.

CORPORATE SOURCE: Sch. Med., UCLA, Los Angeles, CA, 90024, USA

SOURCE: Biochemical Pharmacology (1990), 39(12), 1853-60

DOCUMENT TYPE:

Journal

LANGUAGE:

English

AB In vivo double-labeled expts in rats were designed to correlate the peripheral and cerebral metabolism of 6-[18F]fluoro-L-DOPA ([18F]FDOPA) with that of [3H]L-DOPA. Authentic samples of the major [18F]DOPA metabolites were synthesized to identify the 18F-labeled metabolites. After carbidopa pretreatment and i.v. administration of the compound, the products of peripheral metabolism in plasma were analyzed at times from 3 to 60 min. In the periphery, amine conjugates were detected but they accounted for <15% of the total radioactivity; the major metabolites were 3-O-methyl-6-[18F]fluoro-L-DOPA and 3-O-methyl-[3H]L-DOPA. The rate and extent of 3-O-methylation of [18F]FDOPA exceeded that [3H]L-DOPA. Both 3-O-methylated products entered the striatum and cerebellum where they contributed significant but uniform activity. Anal. of cerebral metabolism in these structures indicated a linear accumulation of total radioactivity: a striatum/cerebellum ratio of 2 was observed by 60 min. 6-[18F]fluorodopamine (35%) and [3H]dopamine (55%) were the major metabolites formed in the striatum; however, the methylated [18F]FDOPA and [3H]DOPA products of predominantly peripheral origin represented 55% (18F) and 35% (3H) of the total radioactivity, resp. Other [3H]dopamine metabolites and their 18F-labeled analogs represented <10-15% at times analyzed. The cerebellum radioactivity was composed only of [18F]FDOPA, [3H]DOPA and their 3-O-methylated products. These data will serve as the basis for the development of kinetic models of [18F]FDOPA metabolism that can be applied to the evaluation of central dopamine biochem. with positron emission tomog. in humans.

IT 31104-98-0, biological studies

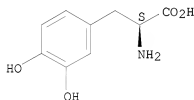
RL: BIOL (Biological study)

(metabolism of fluorodopa vs.)

RN 31104-98-0 CAPLUS

CN L-Tyrosine, 3-hydroxy-, labeled with tritium (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 6 OF 21 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1987:403324 CAPLUS

DOCUMENT NUMBER: 107:3324

TITLE: Cerebral metabolism of 6-[18F]fluoro-L-3,4-dihydroxyphenylalanine in the primate

AUTHOR(S): Firnau, G.; Sood, S.; Chirakal, R.; Nahmias, C.; Garnett, E. S.

CORPORATE SOURCE: Chedoke-McMaster Hosp., McMaster Univ., Hamilton, ON, Can.

SOURCE: Journal of Neurochemistry (1987), 48(4), 1077-82

CODEN: JONRA9; ISSN: 0022-3042

DOCUMENT TYPE:

Journal

LANGUAGE:

English

AB The tracers 6-[18F]fluoro-L-DOPA and L-[14C]DOPA were injected simultaneously into rhesus monkeys, and the time course of their metabolites was measured in the striatum and in the occipital and frontal cortices. In the striatum, 6-[18F]fluoro-L-DOPA was metabolized to 6-[18F]fluorodopamine, 3,4-dihydroxy-6-[18F]fluorophenylacetic acid, and

6-[18F]fluorohomovanillic acid. The metabolite pattern was qual. similar to that of L-[14C]DOPA. 6-[18F]Fluorodopamine was synthesized faster than [14C]dopamine. In the frontal cortex, the major metabolite was also 6-[18F]fluorodopamine or [14C]dopamine. In the occipital cortex, the major metabolite was 3-O-methyl-6-[18F]fluoro-L-DOPA. On the basis of these data, the images obtained with 6-[18F]fluoro-L-DOPA and positron emission tomog. in humans can now be interpreted in neurochem. terms.

IT 108570-54-3

RL: BIOL (Biological study)

(as carbon-14-labeled DOPA metabolite, in brain, fluorine-18-labeled fluoro-DOPA metabolism in relation to)

RN 108570-54-3 CAPLUS

CN L-Tyrosine, 3-hydroxy-, hydrogen sulfate (ester), labeled with carbon-14 (9CI) (CA INDEX NAME)

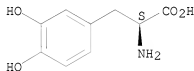
CM 1

CRN 38062-58-7

CMF C9 H11 N O4

CIL XC-14

Absolute stereochemistry.



CM 2

CRN 7664-93-9

CMF H2 O4 S



L5 ANSWER 7 OF 21 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1986:81911 CAPLUS

DOCUMENT NUMBER: 104:81911

ORIGINAL REFERENCE NO.: 104:12849a,12852a

TITLE: Changes in brain catecholamine levels following DL-DOPA are not potentiated by deuterium substitution
AUTHOR(S): Dewar, Karen M.; Dyck, Lillian E.; Durden, David A.; Boulton, A. A.

CORPORATE SOURCE: Psychiatr. Res. Div., Univ. Saskatchewan, Saskatoon, SK, S7N 0W0, Can.

SOURCE: Progress in Neuro-Psychopharmacology & Biological Psychiatry (1985), 9(5-6), 675-80
CODEN: PNPPD7; ISSN: 0278-5846

DOCUMENT TYPE: Journal

LANGUAGE: English

AB In rats treated with either DL-dopa [63-84-3] or its deuterated analog D3-DL-dopa [100364-65-6], total dopamine [51-61-6] levels in the brain striatum increased above control values; however, no differences

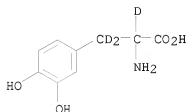
were observed in the effects between these 2 treatments. Total noradrenaline [51-41-2] levels were not significantly altered by treatment with either DL-dopa or D3-DL-dopa. Thus, D substitution does not appear to affect catecholamine deamination or β -hydroxylation in vivo.

IT 100364-65-6

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(catecholamines of brain response to)

RN 100364-65-6 CAPLUS

CN Tyrosine- α,β,β -d3, 3-hydroxy- (9CI) (CA INDEX NAME)



L5 ANSWER 8 OF 21 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1984:403121 CAPLUS

DOCUMENT NUMBER: 101:3121

ORIGINAL REFERENCE NO.: 101:547a,550a

TITLE: Characteristics of kinetics of metabolism and the biological action of tritium-labeled organic compounds
AUTHOR(S): Zhuravlev, V. F.; Kalyazina, N. S.; Klykov, O. V.; Goryacheva, T. I.

CORPORATE SOURCE: USSR

SOURCE: Biol. Effekty Mal. Doz. Radiatsii, M. (1983) 74-7
From: Ref. Zh., Radiats. Biol. 1984, Abstr. No. 270102
DOCUMENT TYPE: Journal
LANGUAGE: Russian

AB Title only translated.

IT 31104-98-0, biological studies

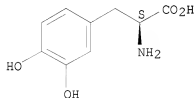
RL: ADV (Adverse effect, including toxicity); BPR (Biological process);
BSU (Biological study, unclassified); BIOL (Biological study); PROC
(Process)

(metabolism and toxicity of)

RN 31104-98-0 CAPLUS

CN L-Tyrosine, 3-hydroxy-, labeled with tritium (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 9 OF 21 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1982:577974 CAPLUS

DOCUMENT NUMBER: 97:177974

ORIGINAL REFERENCE NO.: 97:29695a,29698a

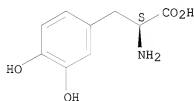
TITLE: Standardization of tritium-labeled compounds

AUTHOR(S): Kalyazina, N. S.; Klykov, O. V.; Zhuravlev, V. F.;

Moskalev, Yu. I.
CORPORATE SOURCE: USSR
SOURCE: Meditsinskaya Radiologiya (1982), 27(8), 53-7
CODEN: MERAA9; ISSN: 0025-8334
DOCUMENT TYPE: Journal
LANGUAGE: Russian

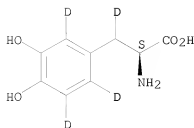
AB The kinetics of the metabolism of tritium in rats following i.p. administration of tritiated organic compds. (thymidine, ethyleneglycol, cytidine, EtOH, glucose, AcOH, and dopa) differed from that of HTO. The rate of removal of tritium administered in an organic compound was slower than that of HTO. Also tissue levels of tritium were higher after administration of the label in organic compds. The toxicity of the organic tritiated compds. was also higher than that of HTO. The half-life constant, absorbed dose, and permissible concns. of tritium in workers exposed to HTO and the above-mentioned tritiated compds. were calculated
IT 31104-98-0, Biological studies
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process) (metabolism and permissible levels of, in humans and laboratory animals)
RN 31104-98-0 CAPLUS
CN L-Tyrosine, 3-hydroxy-, labeled with tritium (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 10 OF 21 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1982:180880 CAPLUS
DOCUMENT NUMBER: 96:180880
ORIGINAL REFERENCE NO.: 96:29795a,29798a
TITLE: Deuterium exchange labeling of biologically important phenols, indoles, and steroids
AUTHOR(S): Vining, R. F.; Smythe, G. A.; Long, M. A.
CORPORATE SOURCE: Garvan Inst. Med. Res., St. Vincent's Hosp., Sydney, 2010, Australia
SOURCE: Journal of Labelled Compounds and Radiopharmaceuticals (1981), 18(11), 1683-92
CODEN: JLCRD4; ISSN: 0362-4803
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Deuterated analogs of phenolic steroids, catechols, and indole derivs. were prepared in high chemical yield by heating the relevant compound in D2O at 190° in a sealed tube for 24 h. E.g., vanillin in D2O gave >95% vanillin-5-d1 almost exclusively. Care must be exercised in the heating of the sealed tubes due to considerable risk of explosion.
IT 81587-02-2P
RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of, by deuterium exchange reaction of parent compound with deuterium oxide)
RN 81587-02-2 CAPLUS
CN L-Tyrosine-β,2,3,6-d4, 5-hydroxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 11 OF 21 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1982:100179 CAPLUS

DOCUMENT NUMBER: 96:100179

ORIGINAL REFERENCE NO.: 96:16401a,16404a

TITLE: Effect of the form of the introduced compound and isotopic carrier on the kinetics of carbon-14, tritium, and iodine-125 metabolism

AUTHOR(S): Moskalev, Yu. I.; Kalistratova, V. S.; Vasilenko, I. Ya.; Bugryshev, P. F.; Kalyazina, N. S.; Zhuravlev, V. F.

CORPORATE SOURCE: Inst. Biofiz., Moscow, USSR

SOURCE: Rep.-SAAS - Staatl. Amt Atomsicherh. Strahlenschutz DDR (1981), SAAS-280, Itogovaya Konf. Nauchno - Tekh. Sotr. Obl. Radiats. Bezop. Minist. Zdravookhr. SSSR Gos. Upr. At. Bezop. Zashch. Izluch. Period 1979 - 1980, 181-96

CODEN: RSADDL; ISSN: 0138-2551

DOCUMENT TYPE: Report

LANGUAGE: Russian

AB The effects of form (organic or inorg.) on the metabolism of ¹⁴C, ³H, and ¹²⁵I in

rats were studied. The inorg. Na²¹⁴CO₃, K²¹⁴CO₃, and Ca¹⁴CO₃ were rapidly absorbed by the gastrointestinal tract and ¹⁴CO₂ was rapidly eliminated via respiration. The organic labeled compds. glucose-¹⁴C, glycine-¹⁴C, and palmitate-¹⁴C were also rapidly absorbed by the intestine, but greater amts. of label were found in tissues, especially after glycine and palmitate administration. Labeling of tissues was also higher following administration of tritiated organic compds. (dopa-³H, [³H]EtOH, glucose-³H, acetate-³H, thymidine-³H, and cytidine-³H) than after tritium oxide administration. Accumulation (30-day) of label from dopa-³H was less by a factor of 3 and that of thymidine-³H was 28-fold greater than that of tritium oxide. In rats, resorption of ¹²⁵I by the gastrointestinal tract was not affected by the presence of the isotope carrier ¹²⁷I; however, incorporation of ¹²⁵I by the thyroid gland was inhibited by the carrier.

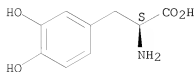
IT 38062-58-7, biological studies

RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process) (metabolism of)

RN 38062-58-7 CAPLUS

CN L-Tyrosine, 3-hydroxy-, labeled with carbon-14 (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 12 OF 21 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1981:1628 CAPLUS

DOCUMENT NUMBER: 94:1628

ORIGINAL REFERENCE NO.: 94:335a,338a

TITLE: Tritiated DOPA: distribution in subcellular melanoma fractions and prospects for its radiotherapeutical use

AUTHOR(S): Gavrilenko, I. S.; Rumyantsev, P. P.; Bulychev, A. G.; Zaremskii, R. A.; Ivanov, I. I.

CORPORATE SOURCE: Lab. Cell. Morphol., Inst. Cytol., Leningrad, USSR

SOURCE: Radiobiologia, Radiotherapia (1980), 21(4), 525-31

CODEN: RDBGAT; ISSN: 0033-8184

DOCUMENT TYPE: Journal

LANGUAGE: German

AB DOPA-3H was prepared and after injection into mice with Harding-Passey melanoma, radioactivity was selectively incorporated into tumor melanosomes and especially mitochondria. The incorporation of label into these 2 tumor cell fractions was associated with increases in tyrosinase activity. The highly selective absorption of DOPA-3H by melanocytes indicates that DOPA may be useful as the carrier of an emitter for the internal radiation therapy of melanoma.

IT 31104-98-0, biological studies

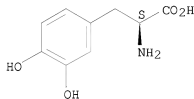
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)

(metabolism of, by melanoma, radiotherapy in relation to)

RN 31104-98-0 CAPLUS

CN L-Tyrosine, 3-hydroxy-, labeled with tritium (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 13 OF 21 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1979:18868 CAPLUS

DOCUMENT NUMBER: 90:18868

ORIGINAL REFERENCE NO.: 90:3087a,3090a

TITLE: Autoradiographic and metabolic studies of

Mycobacterium leprae

AUTHOR(S): Khanolkar, Saroj R.; Ambrose, E. J.; Chulawala, R. G.; Bapat, C. V.

CORPORATE SOURCE: Found. Med. Res., Worli, India

SOURCE: Leprosy Review (1978), 49(3), 187-98

CODEN: LEREAA; ISSN: 0305-7518

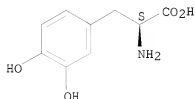
DOCUMENT TYPE: Journal

LANGUAGE: English

AB Highly purified suspensions of M. leprae showed a progressive increase in the incorporation of thymidine-3H and DOPA(I)-3H in short-term cultures as shown by scintillation counting. The intact bacilli are known to have a high permeability barrier. Apparently, I-3H becomes trapped within this barrier and oxidized inside the bacilli. Tests by pretreatment with di-Et diithiocarbamate, an inhibitor of I, cold I, or hyaluronidase distinguished the uptake of I-3H by bacilli from the effects of connective tissue contamination. Similar increases in the labeling of bacilli by scintillation counting were observed by autoradiog. of the organisms. The scintillation method shows promise for rapidly identifying drug resistance in lepromatous patients relapsing while on treatment with dapsone,

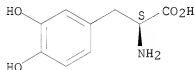
rifampicin, clofazimine, or other anti-leprosy drugs.
 IT 31104-98-0, biological studies
 RL: BIOL (Biological studies)
 (incorporation of, by Mycobacterium leprae, viability assessment by)
 RN 31104-98-0 CAPLUS
 CN L-Tyrosine, 3-hydroxy-, labeled with tritium (9CI) (CA INDEX NAME)

Absolute stereochemistry.



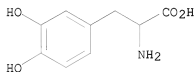
L5 ANSWER 14 OF 21 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1973:402362 CAPLUS
 DOCUMENT NUMBER: 79:2362
 ORIGINAL REFERENCE NO.: 79:439a,442a
 TITLE: Preparation of L-tyrosine-ring-14C, L-dopa- ring-14C, and related metabolites
 AUTHOR(S): Ellis, B. E.; Major, G.; Zenk, M. H.
 CORPORATE SOURCE: Ruhr-Univ., Bochum-Querenburg, Fed. Rep. Ger.
 SOURCE: Analytical Biochemistry (1973), 53(2), 470-7
 CODEN: ANBCA2; ISSN: 0003-2697
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB The reversibility of the tyrosine phenol-lyase reaction was utilized to develop a simple system in which phenol-14C is incorporated into L-tyrosine in high yield. By use of mushroom tyrosinase, catechol-14C can be prepared from phenol-14C and L-dopa-14C from L-tyrosine-14C. Catechol-14C can also be incorporated into L-dopa-14C by use of tyrosine phenol-lyase, giving the possibility of preparing dopa with 2 labeling patterns in the ring when starting from phenol-14C. Two further tyrosine metabolites, p-coumaric acid and homogentisic acid, were also enzymically prepared with 14C in the ring.
 IT 38062-58-7P
 RL: PREP (Preparation)
 (preparation of)
 RN 38062-58-7 CAPLUS
 CN L-Tyrosine, 3-hydroxy-, labeled with carbon-14 (9CI) (CA INDEX NAME)

Absolute stereochemistry.



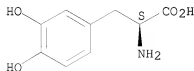
L5 ANSWER 15 OF 21 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1973:148206 CAPLUS
 DOCUMENT NUMBER: 78:148206
 ORIGINAL REFERENCE NO.: 78:23833a,23836a
 TITLE: Possible differential radiolysis of amino acid optical isomers by carbon-14-labeled betas
 AUTHOR(S): Bernstein, William James; Lemmon, Richard M.; Calvin,

Melvin
CORPORATE SOURCE: Lawrence Radiat. Lab., Univ. California, Berkeley, CA, USA
SOURCE: Mol. Evol. (1972), 151-5. Editor(s): Rohlfing, Duane L. Plenum: New York, N. Y.
CODEN: 26NJAU
DOCUMENT TYPE: Conference
LANGUAGE: English
AB No differential radiolysis of the D- and L-isomers was detected in samples of 14C-labeled DL-amino acids irradiated intrinsically by β - particles and their bremsstrahlung derived from the 14C, for 12-24 years. The radiation doses were 2.5-10.4 $\times 10^7$ rads. Norvaline, alanine, DOPA, aspartic acid, and methionine were analyze
IT 40857-06-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(differential radiolysis of isomers in)
RN 40857-06-5 CAPLUS
CN Tyrosine, 3-hydroxy-, labeled with carbon-14 (9CI) (CA INDEX NAME)



L5 ANSWER 16 OF 21 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1972:527015 CAPLUS
DOCUMENT NUMBER: 77:127015
ORIGINAL REFERENCE NO.: 77:20937a,20940a
TITLE: Thin-layer chromatographic separation of optical isomers on labeled dopa via dipeptide formation
AUTHOR(S): Barooshian, Armen V.; Lautenschleger, Margaret J.; Harris, Wayne G.
CORPORATE SOURCE: Anal. Dep., New England Nucl. Corp., Boston, MA, USA
SOURCE: Analytical Biochemistry (1972), 49(2), 569-71
CODEN: ANBCA2; ISSN: 0003-2697
DOCUMENT TYPE: Journal
LANGUAGE: English
AB DL-Dopa-carboxyl-14C reacted with L-leucine-N-carboxy anhydride to give a diastereomeric mixture of L-Leu-D-Dopa-14C (I) and L-Leu-L-Dopa-14C (II). Thin-layer chromatog. of I and II gave Rf 0.38 and 0.56, resp.
IT 38062-58-7
RL: PRP (Properties)
(optical purity of, determination by thin-layer chromatog. of dipeptides of)
RN 38062-58-7 CAPLUS
CN L-Tyrosine, 3-hydroxy-, labeled with carbon-14 (9CI) (CA INDEX NAME)

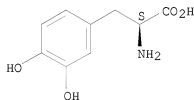
Absolute stereochemistry.



L5 ANSWER 17 OF 21 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1971:72582 CAPLUS
DOCUMENT NUMBER: 74:72582

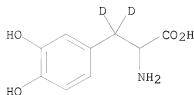
ORIGINAL REFERENCE NO.: 74:11727a
 TITLE: [3H]-Dopa in [3H]-tyrosine with high specific activity: a serious complication in the study of catechol amine metabolism
 AUTHOR(S): Waldeck, Bertil
 CORPORATE SOURCE: Dep. Pharmacol., Univ. Goteborg, Goteborg, Swed.
 SOURCE: Journal of Pharmacy and Pharmacology (1971), 23(1), 64-5
 CODEN: JPPMAB; ISSN: 0022-3573
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI For diagram(s), see printed CA Issue.
 AB The use of 3H-labeled tyrosine (I) with high specific activity, contaminated with 10% 3H-labeled dopa (3,4-dihydroxyphenyl-alanine), for the study of catechol amine metabolism in rats gave abnormally high values for the yields of labeled noradrenaline and dopamine. The levels of radioactive metabolites in heart were most significantly increased by the contamination, as compared with those in the caudate nucleus and the spinal cord.
 IT 31104-98-0
 RL: ANST (Analytical study)
 (catechol amine metabolism studies in response to)
 RN 31104-98-0 CAPLUS
 CN L-Tyrosine, 3-hydroxy-, labeled with tritium (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 18 OF 21 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1970:510104 CAPLUS
 DOCUMENT NUMBER: 73:110104
 ORIGINAL REFERENCE NO.: 73:17935a,17938a
 TITLE: Deuteration and tritiation of aryl aldehydes in the formyl group and the synthesis of (+)-3,4-dihydroxy[β-2H2]phenylalanine
 AUTHOR(S): Bennett, David John; Kriby, G. W.; Moss, V. A.
 CORPORATE SOURCE: Chem. Dep., Univ. Technol., Loughborough, UK
 SOURCE: Journal of the Chemical Society [Section] C: Organic (1970), (15), 2049-51
 CODEN: JSOAX; ISSN: 0022-4952
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 73:110104
 AB Aryl aldehydes were converted into the corresponding α-aryl-α-morpholinoacetonitriles and by treatment with base into the derived benzylic anions. Quenching of these anions with D2O or T2O followed by hydrolysis with mineral acid, gave formyl-labeled aldehydes. 3,4-Dimethoxybenzaldehyde-formyl-d gave, when heated with alkali, 3,4-dimethoxybenzyl-methylene-d2 alc., a convenient starting material for the synthesis of (±)-3,4-dihydroxyphenylalanine-β,β-d2.
 IT 27313-66-2P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
 RN 27313-66-2 CAPLUS

CN Tyrosine- β , β -d₂, 3-hydroxy- (9CI) (CA INDEX NAME)



L5 ANSWER 19 OF 21 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1970:435751 CAPLUS

DOCUMENT NUMBER: 73:35751

ORIGINAL REFERENCE NO.: 73:5933a,5936a

TITLE: Chemistry of melanins. XI. Distribution of the polymeric linkages in dopa-melanin
AUTHOR(S): King, J. A. G.; Percival, A.; Robson, N. C.; Swan, G. A.

CORPORATE SOURCE: Dep. Org. Chem., Univ. Newcastle upon Tyne, Newcastle upon Tyne, UK

SOURCE: Journal of the Chemical Society [Section] C: Organic (1970), (10), 1418-22

CODEN: JSOOAX; ISSN: 0022-4952

DOCUMENT TYPE: Journal

LANGUAGE: English

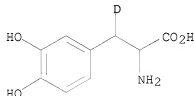
AB Samples of (\pm)-3,4-dihydroxyphenylalanine deuterated at the α -, β -, 2-, 5-, and 6-positions were each converted into melanin, both by autoxidn. and enzymically, and the incorporation of D into these melanins was measured. The results were interpreted in terms of an outline structure suggested for dopa-melanin on the basis of earlier expts.; and the relative nos. of polymeric linkages at different positions of the polymeric units were estimated. No evidence was found that enzymic dopa-melanin was fundamentally different from the autoxidative melanin. Dopa-melanin, prepared in vitro, appears to be an irregular polymer, containing a number of different types of unit, linked in various ways.

IT 27447-24-1

RL: RCT (Reactant); RACT (Reactant or reagent)
(melanin formation from)

RN 27447-24-1 CAPLUS

CN Alanine-3-d, 3-(3,4-dihydroxyphenyl)-, DL- (8CI) (CA INDEX NAME)



L5 ANSWER 20 OF 21 CAPLUS COPYRIGHT 2008 ACS on STN

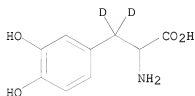
ACCESSION NUMBER: 1970:415200 CAPLUS

DOCUMENT NUMBER: 73:15200

ORIGINAL REFERENCE NO.: 73:2541a,2544a

TITLE: Studies related to the chemistry of melanins. IX. Syntheses of specifically deuteriated 3,4-dihydroxyphenethylamines and (\pm)-3,4-dihydroxyphenylalanines

AUTHOR(S): Binns, F.; King, J. A. G.; Percival, A.; Robson, N. C.; Swan, George A.
 CORPORATE SOURCE: Dep. Org. Chem., Univ. Newcastle upon Tyne, Newcastle upon Tyne, UK
 SOURCE: Journal of the Chemical Society [Section] C: Organic (1970), (8), 1134-8
 CODEN: JSOQAX; ISSN: 0022-4952
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB 3,4-Dihydroxyphenethylamine-HCl and (±)-3,4-dihydroxyphenylalanine deuterated at the α-, β-, 2-, 5, and 6-positions (sep.) were synthesized.
 IT 27313-66-2P
 RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)
 RN 27313-66-2 CAPLUS
 CN Tyrosine-β,β-d₂, 3-hydroxy- (9CI) (CA INDEX NAME)



L5 ANSWER 21 OF 21 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1966:35729 CAPLUS
 DOCUMENT NUMBER: 64:35729
 ORIGINAL REFERENCE NO.: 64:6602a-b
 TITLE: Some studies of the formation and structure of melanins
 AUTHOR(S): Swan, George Albert
 CORPORATE SOURCE: Univ. Newcastle-upon-Tyne, UK
 SOURCE: Rend. Accad. Sci. Fis. Mat. (Soc. Nazl. Sci., Napoli) (1964), 31, 212-31
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB In addition to a literature review on the subject (25 references), studies are described of the formation of melanins (I), (a) enzymically, and (b) by autoxidn. from 2,3-(HO)2C6H3CH2CH(CO2H)NH2 (II) and 2,3-(HO)2C6H3CH2CH2NH2 (III). When II and III were labeled with D in the α or β position of the side chain and then converted to I, large retention of D was observed in the I. This suggests that the I are not polymers composed entirely of indole-5,6-quinone, but that they also contain uncyclized units of the precursors (or quinones derived from these) or (more probably) units of 2,3-dihydroindole-5,6-quinone. When I prepared from II-carboxy-14C was oxidized, the resulting pyrrole-2,3,5-tricarboxylic acid was radioactive while the pyrrole-2,3-dicarboxylic acid was inactive.
 IT 27447-24-1P, Alanine-3-d, 3-(3,4-dihydroxyphenyl)-
 RL: PREP (Preparation) (melanin synthesis from)
 RN 27447-24-1 CAPLUS
 CN Alanine-3-d, 3-(3,4-dihydroxyphenyl)-, DL- (8CI) (CA INDEX NAME)

